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* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JUL 02	LMEDLINE coverage updated
NEWS	3	JUL 02	SCISEARCH enhanced with complete author names
NEWS	4	JUL 02	CHEMCATS accession numbers revised
NEWS	5	JUL 02	CA/CAPplus enhanced with utility model patents from China
NEWS	6	JUL 16	CAplus enhanced with French and German abstracts
NEWS	7	JUL 18	CA/CAPplus patent coverage enhanced
NEWS	8	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS	9	JUL 30	USGENE now available on STN
NEWS	10	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS	11	AUG 06	FSTA enhanced with new thesaurus edition
NEWS	12	AUG 13	CA/CAPplus enhanced with additional kind codes for granted patents
NEWS	13	AUG 20	CA/CAPplus enhanced with CAS indexing in pre-1907 records
NEWS	14	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS	15	AUG 27	USPATOLD now available on STN
NEWS	16	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS	17	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS	18	SEP 13	FORIS renamed to SOFIS
NEWS	19	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS	20	SEP 17	CA/CAPplus enhanced with printed CA page images from 1967-1998
NEWS	21	SEP 17	CAplus coverage extended to include traditional medicine patents
NEWS	22	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	23	OCT 02	CA/CAPplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS	24	OCT 19	BEILSTEIN updated with new compounds
NEWS EXPRESS	19	SEPTEMBER 2007:	CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS LOGIN			Welcome Banner and News Items
NEWS IPC8			For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 13:41:29 ON 22 OCT 2007

=> file registry

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 13:42:11 ON 22 OCT 2007

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 OCT 2007 HIGHEST RN 951118-42-6

DICTIONARY FILE UPDATES: 19 OCT 2007 HIGHEST RN 951118-42-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

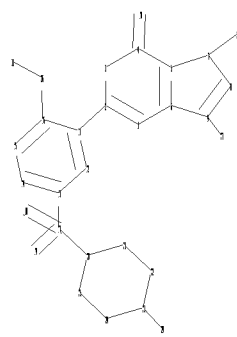
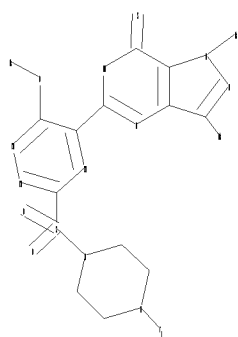
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10 series\10583335\10583335a.str



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chain nodes :
10 17 18 19 26 27 28 29 31
ring nodes :
1 2 3 4 5 6 7 8 9 11 12 13 14 15 16 20 21 22 23 24 25
chain bonds :
2-11 4-10 7-28 9-27 13-17 16-26 17-18 17-19 17-20 23-29 26-31
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 11-12 11-16 12-13 13-14 14-15
15-16 20-21 20-25 21-22 22-23 23-24 24-25
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 4-10 5-6 5-7 6-9 7-8 7-28 8-9 9-27 13-17 16-26
17-18 17-19 17-20 20-21 20-25 21-22 22-23 23-24 23-29 24-25 26-31
exact bonds :
2-11
normalized bonds :

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11-12 11-16 12-13 13-14 14-15 15-16

G1:H,Ak,Cb

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS 28:CLASS
29:CLASS 31:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 13:43:09 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 89 TO ITERATE

100.0% PROCESSED 89 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1214 TO 2346

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 13:43:13 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1639 TO ITERATE

100.0% PROCESSED 1639 ITERATIONS

25 ANSWERS

SEARCH TIME: 00.00.01

L3 25 SEA SSS FUL L1

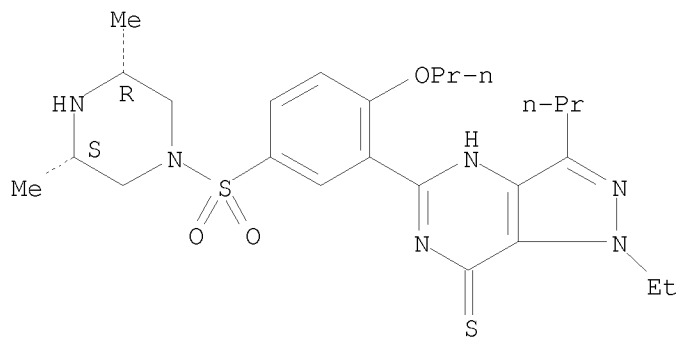
=> d scan

L3 25 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Piperazine, 1-[[3-(1-ethyl-4,7-dihydro-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-propoxyphenyl]sulfonyl]-3,5-dimethyl-, (3R,5S)-rel-(9CI)

MF C25 H36 N6 O3 S2

Relative stereochemistry.

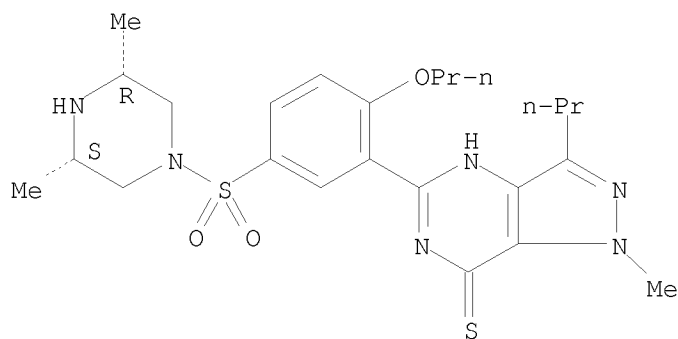


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L3 25 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-propoxyphenyl]sulfonyl]-3,5-dimethyl-, (3R,5S)-rel-
 (9CI)
 MF C24 H34 N6 O3 S2

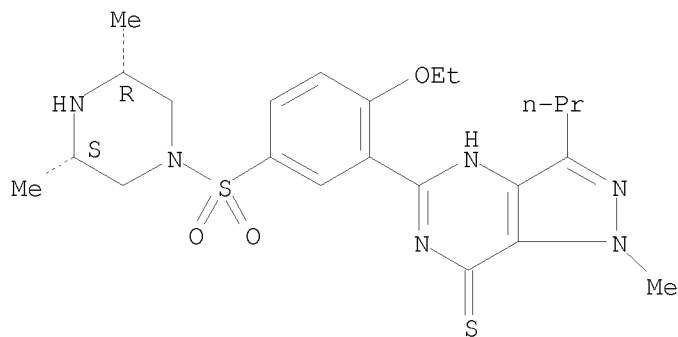
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

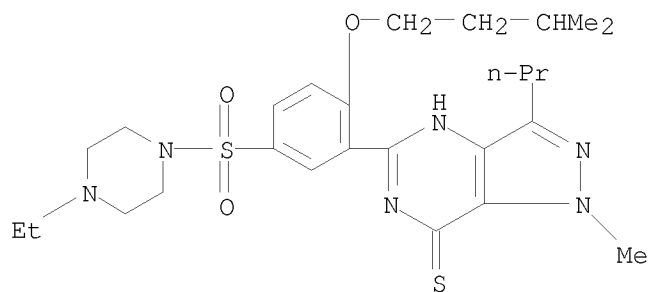
L3 25 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-3,5-dimethyl-, (3R,5S)-rel-
 (9CI)
 MF C23 H32 N6 O3 S2
 CI COM

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 25 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-
 d]pyrimidin-5-yl)-4-(3-methylbutoxy)phenyl]sulfonyl]-4-ethyl- (9CI)
 MF C26 H38 N6 O3 S2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

173.00

173.21

FILE 'CAPLUS' ENTERED AT 13:43:52 ON 22 OCT 2007

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FILE LAST UPDATED: 21 Oct 2007 (20071021/ED)

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<http://www.cas.org/infopolicy.html>

=> s 13

L4 4 L3

=> d 14 1-4 ibib abs hitstr

L4 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:570896 CAPLUS

DOCUMENT NUMBER: 143:97390

TITLE: Preparation of pyrazolopyrimidinethione derivatives for treatment of impotence

INVENTOR(S): Li, Shuxin; Ren, Jianping; Zhao, Yanjin; Lv, Qiu jun; Guo, Jinhua

PATENT ASSIGNEE(S): The Institute of Radiation Medicine, Academy of Military Medical Sciences Pla, Peop. Rep. China

SOURCE: PCT Int. Appl., 34 pp.

CODEN: PIXXD2

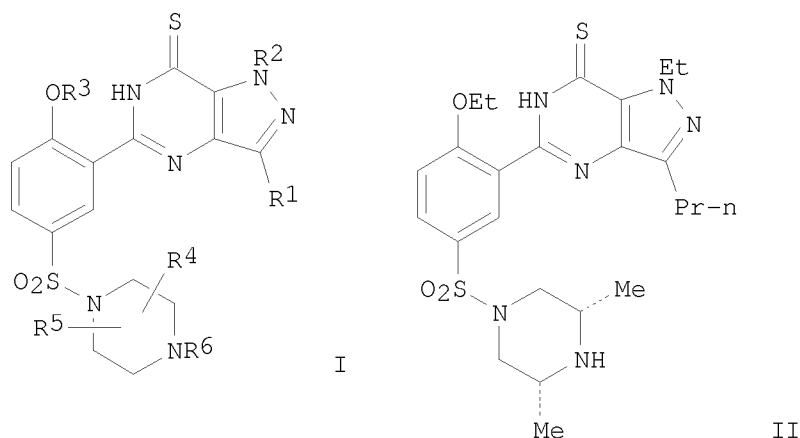
DOCUMENT TYPE: Patent

LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2005058899	A1	20050630	WO 2004-CN1312	20041118
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CN 1629163	A	20050622	CN 2003-10118481	20031218
EP 1695976	A1	20060830	EP 2004-797343	20041118
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
IN 2006MN00737	A	20070330	IN 2006-MN737	20060623
US 2007219220	A1	20070920	US 2007-583335	20070215
PRIORITY APPLN. INFO.:			CN 2003-10118481	A 20031218
			WO 2004-CN1312	W 20041118
OTHER SOURCE(S):		CASREACT 143:97390; MARPAT 143:97390		
GI				



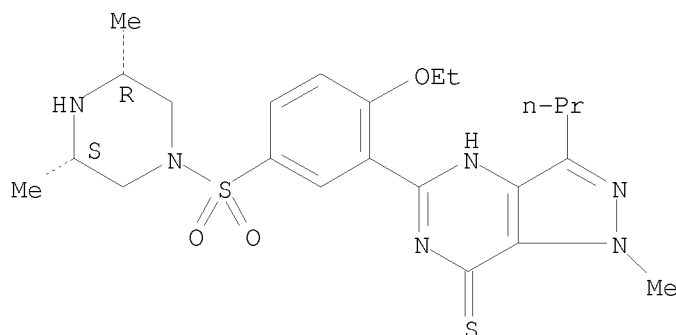
AB Title compds. represented by the formula I [wherein R1-R3 = independently ((cyclo)alkoxy)alkyl, alkenyl or aryl; R4 = alkyl, alkenyl, (cyclo)alkoxy, aryl; R5 = H, alkyl, alkenyl, (cyclo)alkoxy, aryl; R6 = H, (cyclo)alkyl, alkenyl, alkylcarbonyl; and pharmaceutically acceptable salts or solvates thereof] were prepared for treatment of impotence. For example, II was given in a multi-step synthesis starting from 4-amino-1-ethyl-3-propylpyrazole-5-carboxamide. I showed enhanced erectile response in rats similar to that of Sildenafil. Thus, I and their pharmaceutical compns. are useful for the treatment of impotence and sexlessness, having high selectivity over PDE V, long action time, less side reactions, and no side effects of blood pressure decreasing and heart rate increasing.

IT 856190-47-1P
 RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of pyrazolopyrimidinethione derivs. for treatment of impotence)

RN 856190-47-1 CAPLUS

CN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-3,5-dimethyl-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

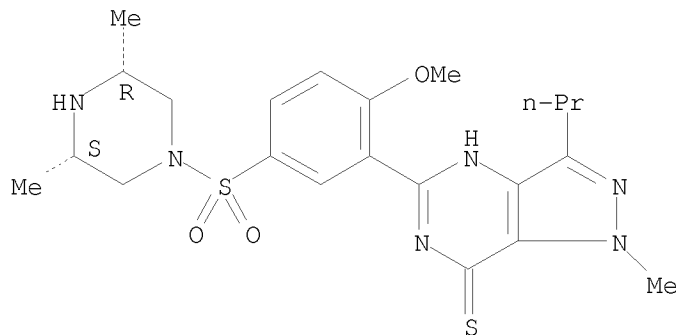


IT 856190-48-2P 856190-49-3P 856190-50-6P
 856190-51-7P 856190-56-2P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of pyrazolopyrimidinethione derivs. for treatment of impotence)

RN 856190-48-2 CAPLUS

CN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-methoxyphenyl]sulfonyl]-3,5-dimethyl-, (3R,5S)-rel-
(9CI) (CA INDEX NAME)

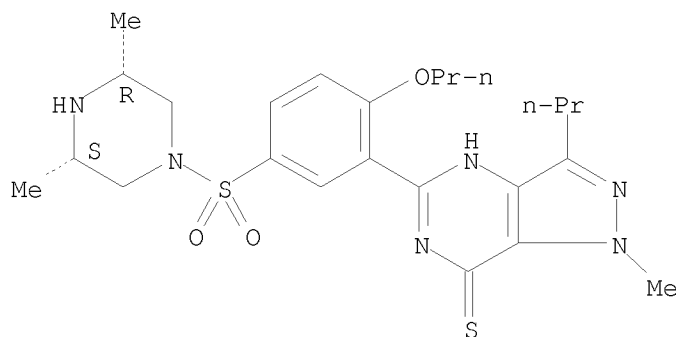
Relative stereochemistry.



RN 856190-49-3 CAPLUS

CN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-propoxyphenyl]sulfonyl]-3,5-dimethyl-, (3R,5S)-rel-
(9CI) (CA INDEX NAME)

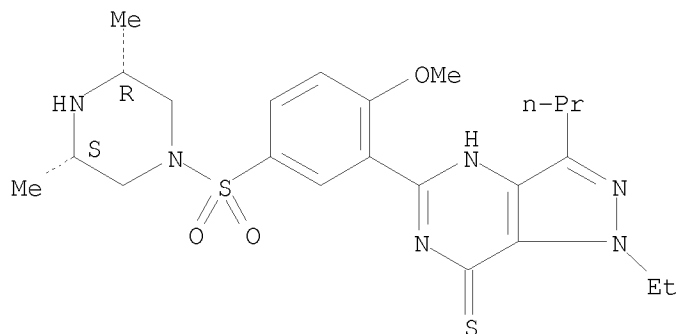
Relative stereochemistry.



RN 856190-50-6 CAPLUS

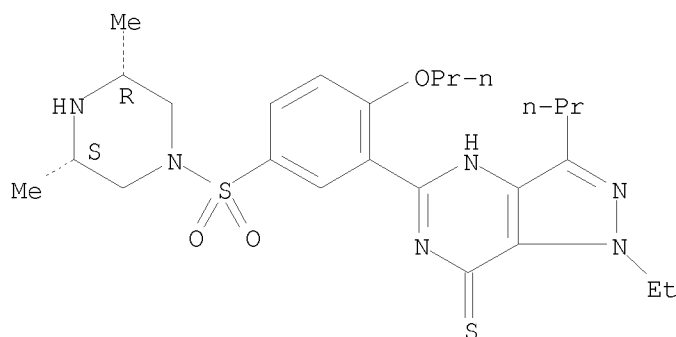
CN Piperazine, 1-[[3-(1-ethyl-4,7-dihydro-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-methoxyphenyl]sulfonyl]-3,5-dimethyl-, (3R,5S)-rel-
(9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 856190-51-7 CAPLUS
 CN Piperazine, 1-[[3-(1-ethyl-4,7-dihydro-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-propoxyphenyl]sulfonyl]-3,5-dimethyl-, (3R,5S)-rel-
 (9CI) (CA INDEX NAME)

Relative stereochemistry.

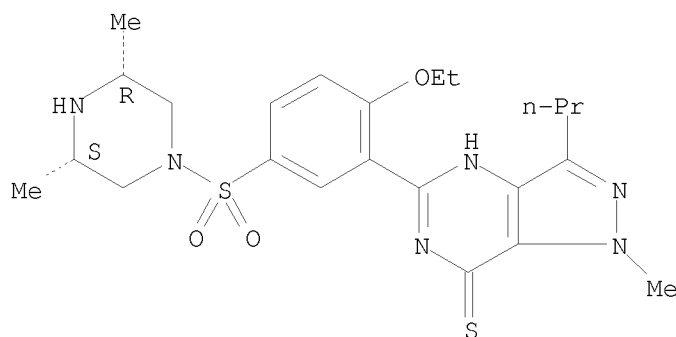


RN 856190-56-2 CAPLUS
 CN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-3,5-dimethyl-, (3R,5S)-rel-,
 2-hydroxy-1,2,3-propanetricarboxylate (1:1) (9CI) (CA INDEX NAME)

CM 1

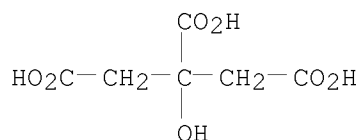
CRN 856190-47-1
 CMF C23 H32 N6 O3 S2

Relative stereochemistry.



CM 2

CRN 77-92-9
 CMF C6 H8 O7



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:565628 CAPLUS

DOCUMENT NUMBER: 143:211579

TITLE: Low-energy collision-induced dissociation of sildenafil thiono analogues: Gas-phase intramolecular nucleophilic substitution through ion-neutral complexes between a cationic substrate and a thione-containing neutral nucleophile

AUTHOR(S): Lee, Jaeick; Yoo, Hye Hyan; Kang, Min-Yung; Kim, Dong-Hyun

CORPORATE SOURCE: Bioanalysis and Biotransformation Research Center, Korea Institute of Science and Technology, Seoul, S. Korea

SOURCE: Rapid Communications in Mass Spectrometry (2005), 19(12), 1767-1770

CODEN: RCMSEF; ISSN: 0951-4198

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Collisional-activation mass spectrometry of sildenafil [i.e., 1-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-(methyl)piperazine] and its thioxo analogs [e.g., 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-(methyl)piperazine] were reported.

IT 479073-72-8 479073-74-0 479073-79-5

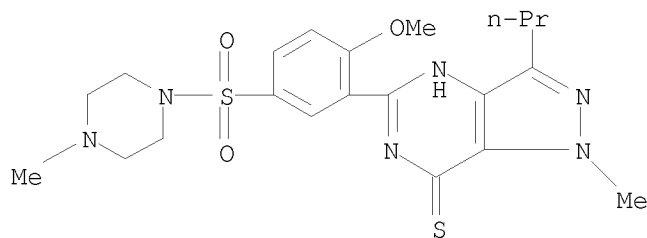
479073-80-8 479073-86-4

RL: PRP (Properties)

(study of low energy collision-induced dissociation of sildenafil and its thioxo analogs and study of gas-phase intramol. nucleophilic substitution through ion-neutral complexes between cationic substrate and thione-containing neutral nucleophile)

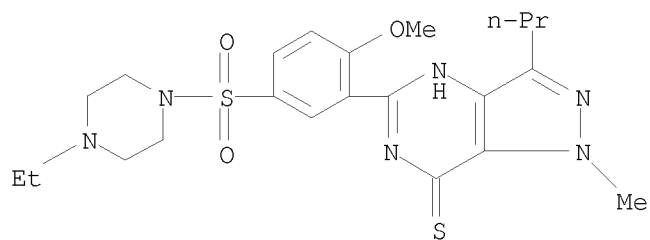
RN 479073-72-8 CAPLUS

CN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-methoxyphenyl]sulfonyl]-4-methyl- (9CI) (CA INDEX NAME)



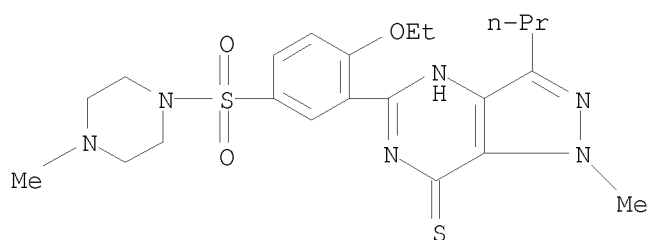
RN 479073-74-0 CAPLUS

CN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-methoxyphenyl]sulfonyl]-4-ethyl- (9CI) (CA INDEX NAME)



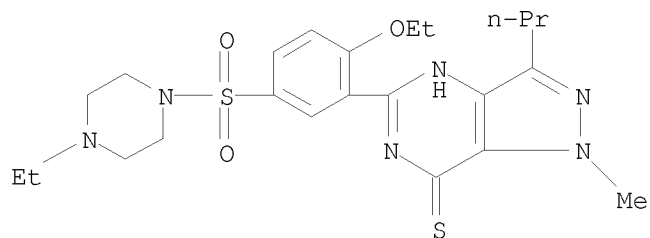
RN 479073-79-5 CAPLUS

CN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methyl- (9CI) (CA INDEX NAME)



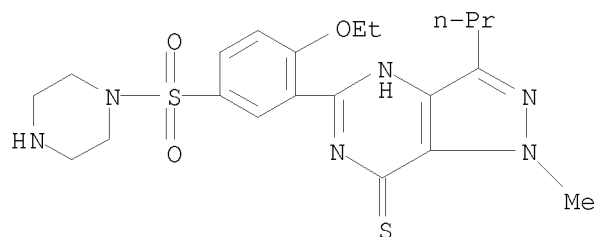
RN 479073-80-8 CAPLUS

CN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-ethyl- (9CI) (CA INDEX NAME)



RN 479073-86-4 CAPLUS

CN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:524375 CAPLUS

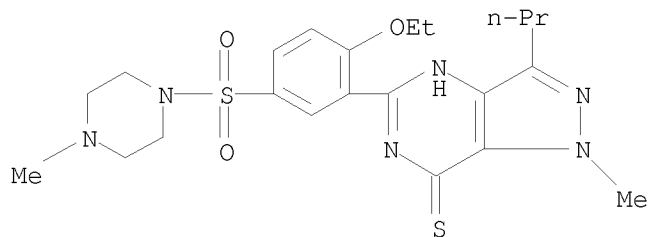
DOCUMENT NUMBER: 141:420374
TITLE: Effects of a new selective phosphodiesterase type 5 inhibitor, KJH-1002, on the relaxation of rabbit corpus cavernosum tissue
AUTHOR(S): Cho, Eun Young; Chung, Sung-Hyun; Kim, Joong Hyup; Kim, Dong-Kyun; Jin, Changbae
CORPORATE SOURCE: Bioanalysis & Biotransformation Research Center, Korea Institute of Science and Technology, Seoul, 130-650, S. Korea
SOURCE: Journal of Applied Pharmacology (2003), 11(4), 232-237
CODEN: JOAPA6; ISSN: 1225-6110
PUBLISHER: Korean Society of Applied Pharmacology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The present study examined functional effects of a new selective phosphodiesterase type 5 inhibitor, 1-[4-ethoxy-3-(6,7-dihydro-1-methyl-7-thioxo-3-propyl-1H-pyrazolo[4,3-pyrimidin-5-yl)phenylsulfonyl]-4-Me piperazine (KJH-1002), in the isolated rabbit corpus cavernosum (RCC). Relaxing effects of KJH-1002 were also compared with those of sildenafil, which is currently used as an oral therapy for penile erectile dysfunction. In the isolated RCC precontracted with phenylephrine, both KJH-1002 and sildenafil in the concentration range of 1 to 1000 nM, produced a comparable potentiation of the elec. field stimulation-induced relaxation in a concentration-dependent manner. In the sodium nitroprusside (SNP)-induced relaxation, the IC50 values, concns. of SNP required to produce a 50% relaxation of the phenylephrine-induced contraction, were significantly decreased to the similar extent by treatments with KJH-1002 and sildenafil. The results suggest that a new selective phosphodiesterase type 5 inhibitor, KJH-1002, has an augmentative effect on penile erection comparable to that of sildenafil and can be useful for the treatment of erectile dysfunction.

IT 479073-79-5
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(KJH-1002 phosphodiesterase type-5 inhibitor produced relaxing effect on rabbit corpus cavernosum and showed augmentative effect on penile erection comparable to that of sildenafil and may be useful in erectile dysfunction treatment)

RN 479073-79-5 CAPLUS

CN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:977816 CAPLUS

DOCUMENT NUMBER: 138:55978

TITLE: Preparation of novel pyrazolopyrimidinethiones as phosphodiesterase V inhibitors for treating erectile

dysfunction

INVENTOR(S): Kim, Joong-Hyup; Kim, Youseung; Choi, Kyung Il; Kim, Dong Hyun; Nam, Ghilsoo; Seo, Jae Hong

PATENT ASSIGNEE(S): Korea Institute of Science and Technology, S. Korea

SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2

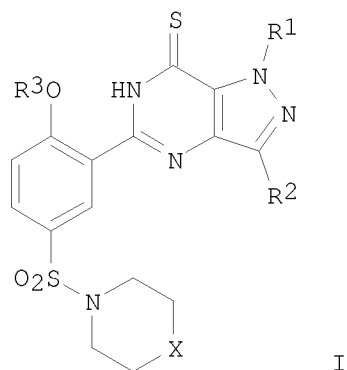
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002102802	A1	20021227	WO 2002-KR1126	20020614
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
KR 2002095286	A	20021226	KR 2001-33382	20010614
AU 2002315822	A1	20030102	AU 2002-315822	20020614
EP 1395593	A1	20040310	EP 2002-741455	20020614
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2005505509	T	20050224	JP 2003-506275	20020614
US 2004176371	A1	20040909	US 2003-480191	20031209
PRIORITY APPLN. INFO.:			KR 2001-33382	A 20010614
			WO 2002-KR1126	W 20020614
OTHER SOURCE(S):			CASREACT 138:55978; MARPAT 138:55978	
GI				



AB The title compds. [I; R1, R2 = H, alkyl, cycloalkyl; R3 = alkyl, cycloalkyl or alkenyl which is unsubstituted or substituted; X = O, NR4; R4 = H, alkyl, cycloalkyl or alkenyl which is unsubstituted or substituted with OH or alkoxy] which exhibit higher inhibitory activities against phosphodiesterase V as well as lower inhibitory activities against phosphodiesterase isoenzymes I, III and VI (biol. data given) and therefore are useful for the treatment of erectile dysfunction, were prepared E.g., a 3-step synthesis of I [R1 = Me; R2 = Pr; R3 = Et; X =

NMe], starting from 5-(2-ethoxyphenyl)-1-methyl-3-propyl-1,6-dihydropyrazolo[4,3-d]pyrimidin-7-one, which showed IC50 of 0.59 nM against PDE V, was given.

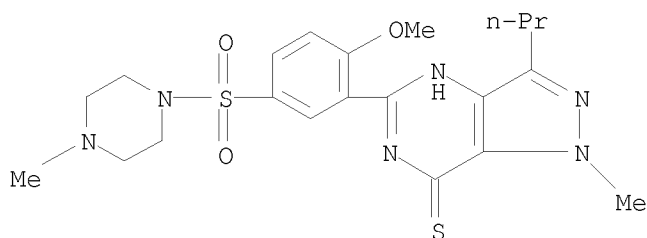
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 479073-94-4P 479073-96-6P 479073-97-7P
 479073-98-8P 479074-00-5P 479074-01-6P
 479074-02-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of novel pyrazolopyrimidinethiones as PDE5 inhibitors for treating erectile dysfunction)

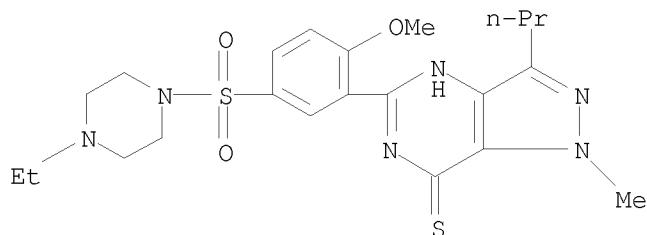
RN 479073-72-8 CAPLUS

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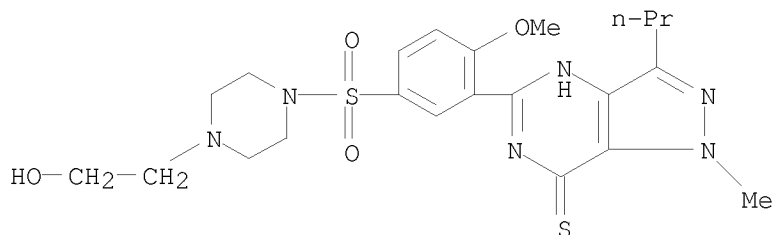
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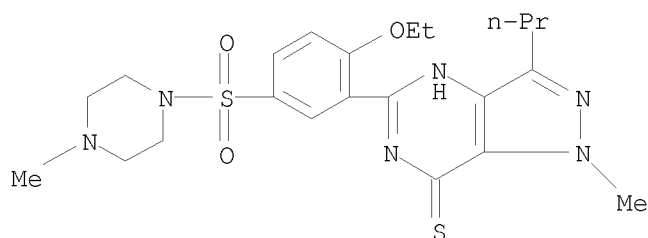


RN 479073-76-2 CAPLUS

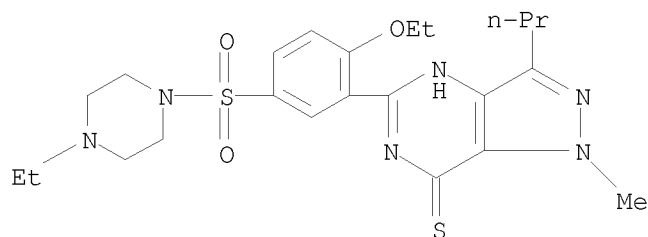
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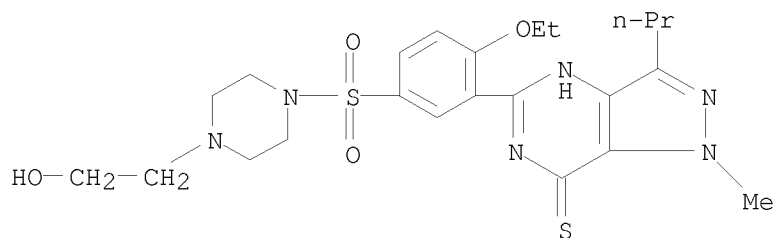
RN 479073-79-5 CAPLUS
 CN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methyl- (9CI) (CA INDEX NAME)



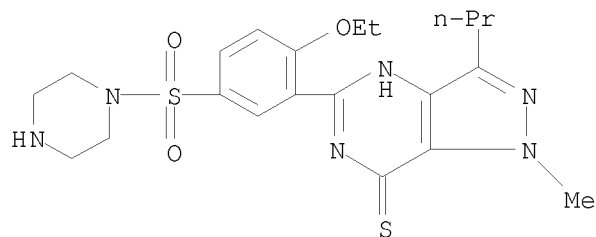
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 CN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-ethyl- (9CI) (CA INDEX NAME)



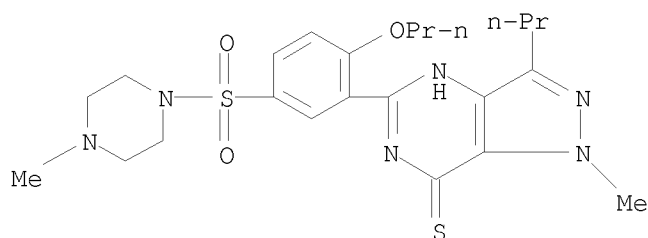
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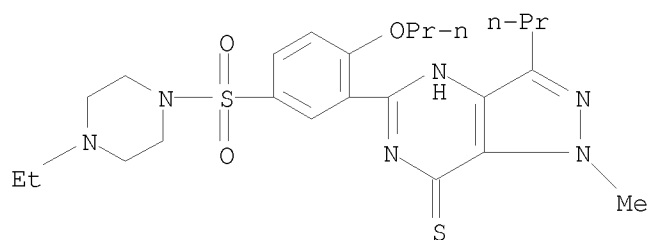
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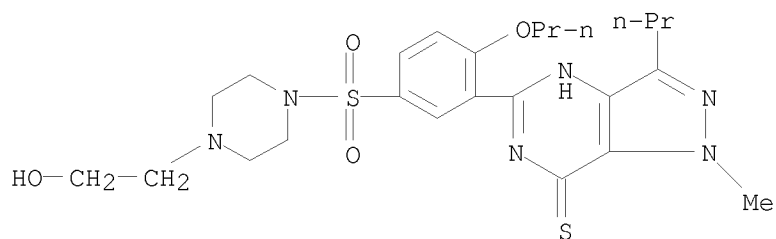
RN 479073-87-5 CAPLUS
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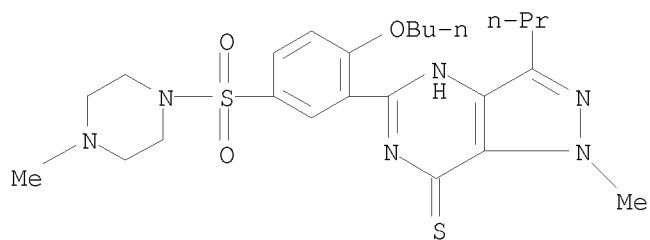
RN 479073-88-6 CAPLUS
 CN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-propoxyphenyl]sulfonyl]-4-ethyl- (9CI) (CA INDEX NAME)



RN 479073-90-0 CAPLUS
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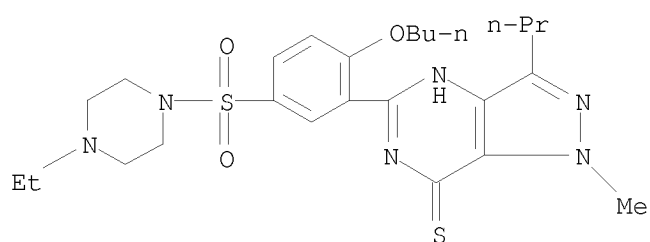


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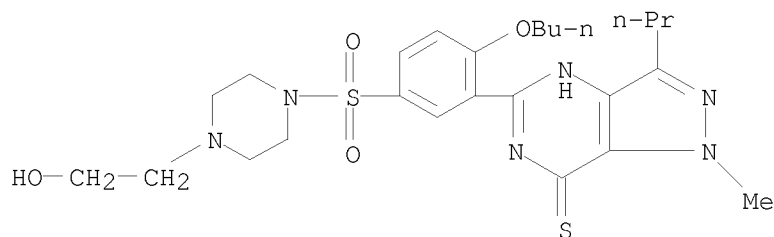
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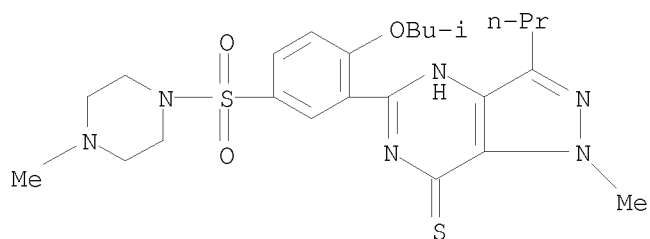
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CN 1-Piperazineethanol, 4-[[4-butoxy-3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



RN 479073-96-6 CAPLUS

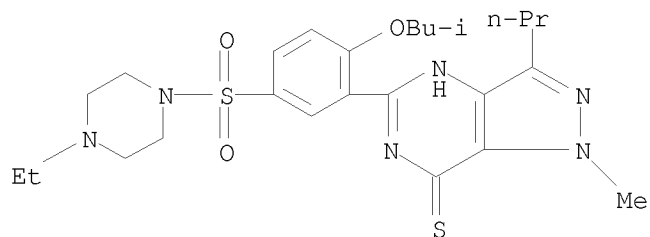
CN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-(2-methylpropoxy)phenyl]sulfonyl]-4-methyl- (9CI) (CA INDEX NAME)



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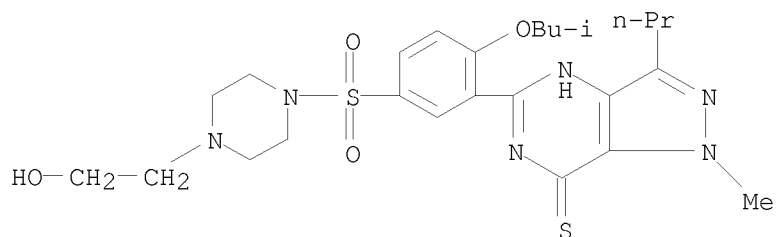
CN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-(2-methylpropoxy)phenyl]sulfonyl]-4-ethyl- (9CI) (CA

INDEX NAME)



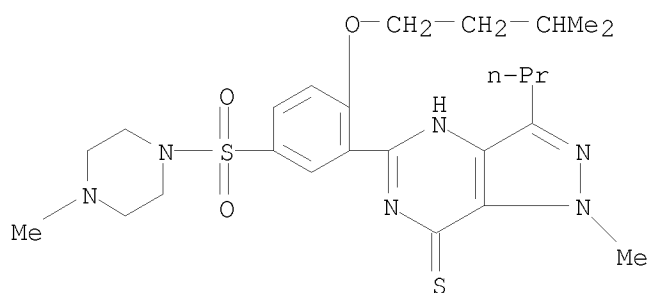
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CN 1-Piperazineethanol, 4-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-(2-methylpropoxy)phenyl]sulfonyl]- (9CI)
(CA INDEX NAME)



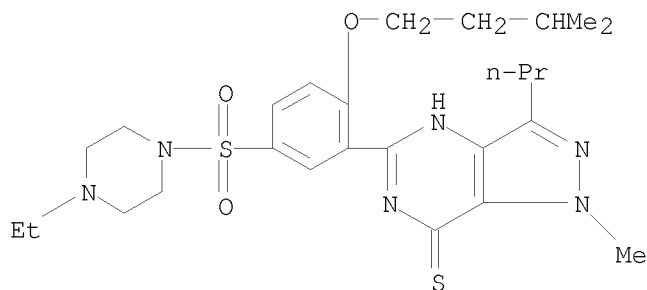
RN 479074-00-5 CAPLUS

CN Piperazine, 1-[[3-(4,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-(3-methylbutoxy)phenyl]sulfonyl]-4-methyl- (9CI) (CA INDEX NAME)

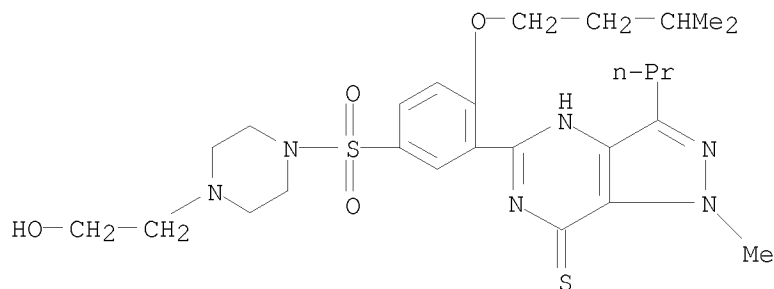


RN 479074-01-6 CAPLUS

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RN 479074-02-7 CAPLUS
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 (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log hold		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	27.19	200.40
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
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CA SUBSCRIBER PRICE	-3.12	-3.12

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 NEWS 2 JUL 02 LMEDLINE coverage updated
 NEWS 3 JUL 02 SCISEARCH enhanced with complete author names
 NEWS 4 JUL 02 CHEMCATS accession numbers revised
 NEWS 5 JUL 02 CA/CAPplus enhanced with utility model patents from China
 NEWS 6 JUL 16 CAPplus enhanced with French and German abstracts
 NEWS 7 JUL 18 CA/CAPplus patent coverage enhanced
 NEWS 8 JUL 26 USPATFULL/USPAT2 enhanced with IPC reclassification
 NEWS 9 JUL 30 USGENE now available on STN
 NEWS 10 AUG 06 CAS REGISTRY enhanced with new experimental property tags
 NEWS 11 AUG 06 FSTA enhanced with new thesaurus edition
 NEWS 12 AUG 13 CA/CAPplus enhanced with additional kind codes for granted patents
 NEWS 13 AUG 20 CA/CAPplus enhanced with CAS indexing in pre-1907 records
 NEWS 14 AUG 27 Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
 NEWS 15 AUG 27 USPATOLD now available on STN
 NEWS 16 AUG 28 CAS REGISTRY enhanced with additional experimental spectral property data
 NEWS 17 SEP 07 STN AnaVist, Version 2.0, now available with Derwent World Patents Index
 NEWS 18 SEP 13 FORIS renamed to SOFIS
 NEWS 19 SEP 13 INPADOCDB enhanced with monthly SDI frequency
 NEWS 20 SEP 17 CA/CAPplus enhanced with printed CA page images from 1967-1998
 NEWS 21 SEP 17 CAPplus coverage extended to include traditional medicine patents
 NEWS 22 SEP 24 EMBASE, EMBAL, and LEMBASE reloaded with enhancements
 NEWS 23 OCT 02 CA/CAPplus enhanced with pre-1907 records from Chemisches Zentralblatt
 NEWS 24 OCT 19 BEILSTEIN updated with new compounds

 NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

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=> file registry

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FULL ESTIMATED COST	0.21	0.21

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DICTIONARY FILE UPDATES: 21 OCT 2007 HIGHEST RN 951124-19-9

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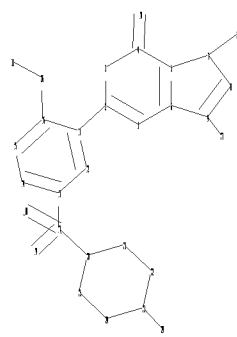
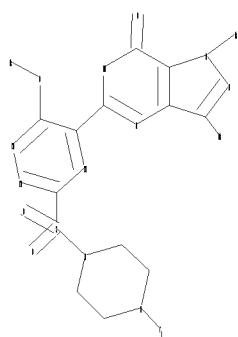
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<http://www.cas.org/support/stngen/stndoc/properties.html>

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ring nodes :
1 2 3 4 5 6 7 8 9 11 12 13 14 15 16 20 21 22 23 24 25
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ring bonds :
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15-16 20-21 20-25 21-22 22-23 23-24 24-25
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 4-10 5-6 5-7 6-9 7-8 7-28 8-9 9-27 13-17 16-26
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exact bonds :
2-11
normalized bonds :

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11-12 11-16 12-13 13-14 14-15 15-16

G1:H,Ak,Cb

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS 28:CLASS
29:CLASS 31:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 10:03:44 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 89 TO ITERATE

100.0% PROCESSED 89 ITERATIONS

9 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1214 TO 2346

PROJECTED ANSWERS: 9 TO 360

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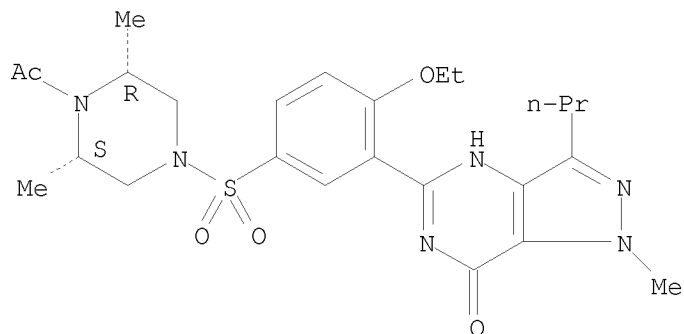
=> d scan

L2 9 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Piperazine, 1-acetyl-4-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-2,6-dimethyl-, (2R,6S)-rel- (9CI)

MF C25 H34 N6 O5 S

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s l1 full

FULL SEARCH INITIATED 10:04:03 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1639 TO ITERATE

100.0% PROCESSED 1639 ITERATIONS

218 ANSWERS

SEARCH TIME: 00.00.01

L3 218 SEA SSS FUL L1

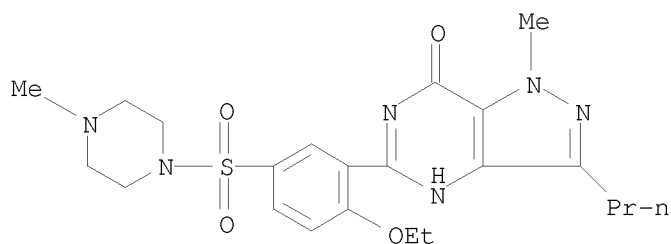
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L3 218 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

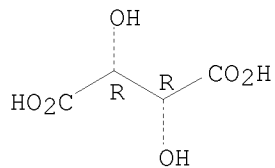
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CM 1



CM 2

Absolute stereochemistry.

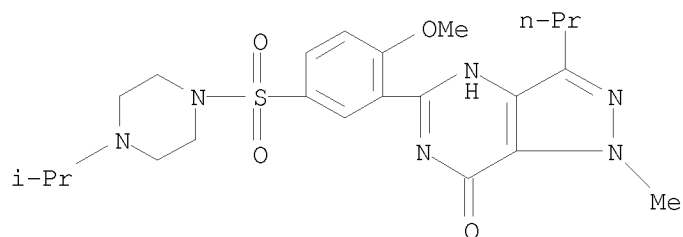


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L3 218 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

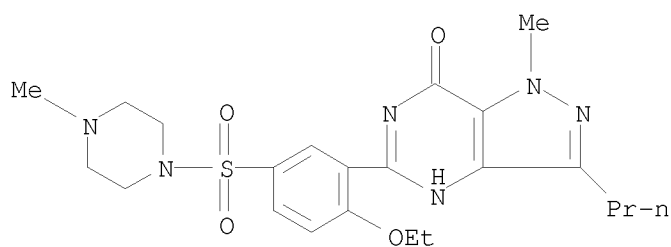
IN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 1,6-dihydro-5-[2-methoxy-5-[[4-(1-methylethyl)-1-piperazinyl]sulfonyl]phenyl]-1-methyl-3-propyl-

MF C23 H32 N6 O4 S

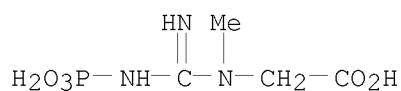


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 218 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN Glycine, N-[imino(phosphonoamino)methyl]-N-methyl-, compd. with
 5-[2-ethoxy-5-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-
 methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one (1:1)
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 CM 1

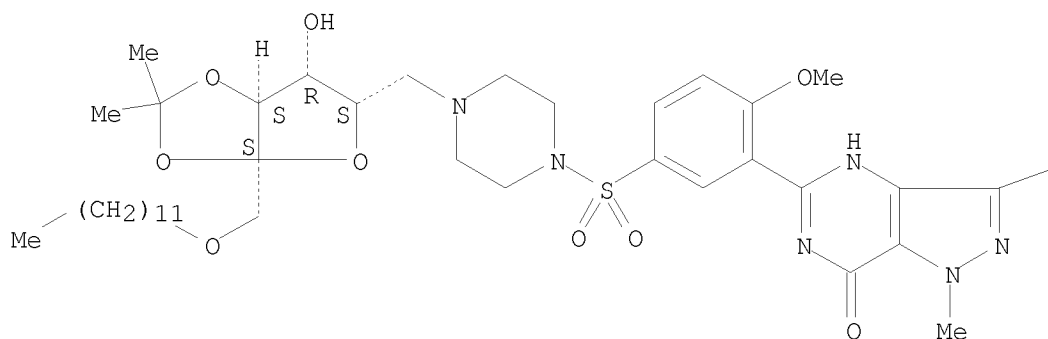


CM 2



L3 218 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN α -L-Sorbofuranose, 6-deoxy-6-[4-[[3-(6,7-dihydro-1-methyl-7-oxo-3-
 propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-methoxyphenyl]sulfonyl]-1-
 piperazinyl]-1-O-dodecyl-2,3-O-(1-methylethylidene)-, hydrochloride (1:1)
 MF C41 H64 N6 O9 S . C1 H

Absolute stereochemistry.



● HCl

Pr-n

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

172.55

172.76

FILE 'CAPLUS' ENTERED AT 10:04:30 ON 23 OCT 2007

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FILE COVERS 1907 - 23 Oct 2007 VOL 147 ISS 18

FILE LAST UPDATED: 22 Oct 2007 (20071022/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 13

L4 1875 L3

=> s 13 not pd>20031218

1875 L3

4864415 PD>20031218

(PD>20031218)

L5 650 L3 NOT PD>20031218

=> file registry

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

3.42

176.18

FILE 'REGISTRY' ENTERED AT 10:06:07 ON 23 OCT 2007

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provided by InfoChem.

STRUCTURE FILE UPDATES: 21 OCT 2007 HIGHEST RN 951124-19-9

DICTIONARY FILE UPDATES: 21 OCT 2007 HIGHEST RN 951124-19-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

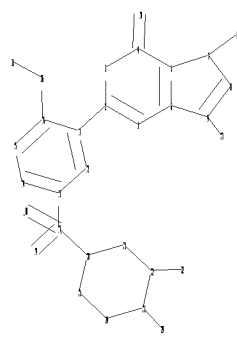
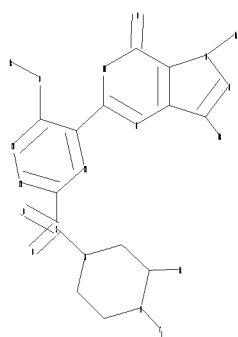
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
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<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10 series\10583335\10583335c.str



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chain nodes :
10 17 18 19 26 27 28 29 31 32
ring nodes :
1 2 3 4 5 6 7 8 9 11 12 13 14 15 16 20 21 22 23 24 25
chain bonds :
2-11 4-10 7-28 9-27 13-17 16-26 17-18 17-19 17-20 22-32 23-29 26-31
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 11-12 11-16 12-13 13-14 14-15
15-16 20-21 20-25 21-22 22-23 23-24 24-25
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 4-10 5-6 5-7 6-9 7-8 7-28 8-9 9-27 13-17 16-26
17-18 17-19 17-20 20-21 20-25 21-22 22-23 22-32 23-24 23-29 24-25 26-31
exact bonds :
2-11
normalized bonds :

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11-12 11-16 12-13 13-14 14-15 15-16

G1:H,Ak,Cb

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS 28:CLASS
29:CLASS 31:CLASS 32:CLASS

L6 STRUCTURE UPLOADED

=> d 16

L6 HAS NO ANSWERS

L6 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 16

SAMPLE SEARCH INITIATED 10:06:28 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 89 TO ITERATE

100.0% PROCESSED 89 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1214 TO 2346

PROJECTED ANSWERS: 1 TO 80

L7 1 SEA SSS SAM L6

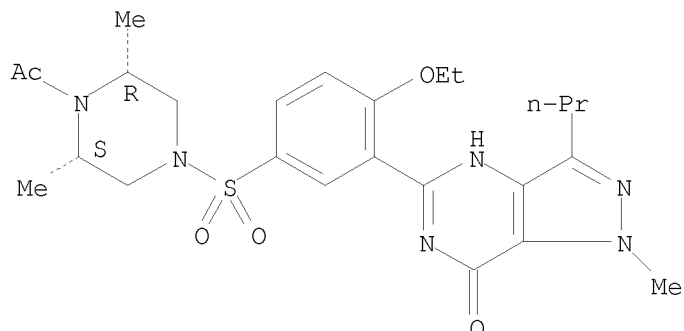
=> d scan

L7 1 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Piperazine, 1-acetyl-4-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-2,6-dimethyl-, (2R,6S)-rel- (9CI)

MF C25 H34 N6 O5 S

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s 16 full

FULL SEARCH INITIATED 10:07:01 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1639 TO ITERATE

100.0% PROCESSED 1639 ITERATIONS

6 ANSWERS

SEARCH TIME: 00.00.01

L8 6 SEA SSS FUL L6

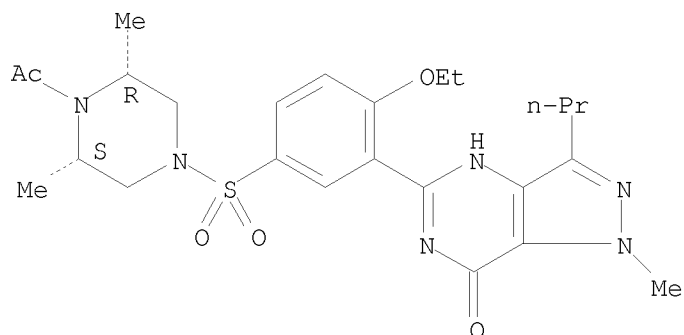
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L8 6 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Piperazine, 1-acetyl-4-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-2,6-dimethyl-, (2R,6S)-rel- (9CI)

MF C25 H34 N6 O5 S

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

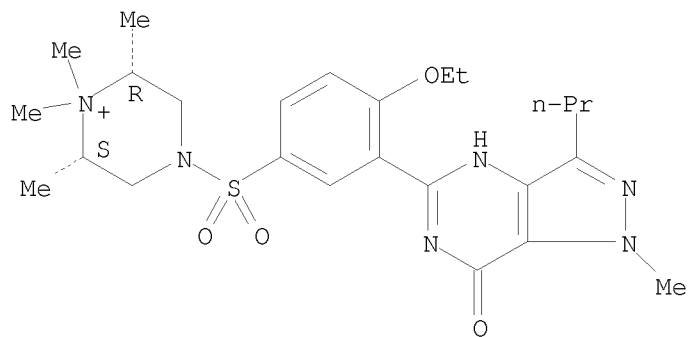
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L8 6 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Piperazinium, 4-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-1,1,2,6-tetramethyl-, (2R,6S)-rel- (9CI)

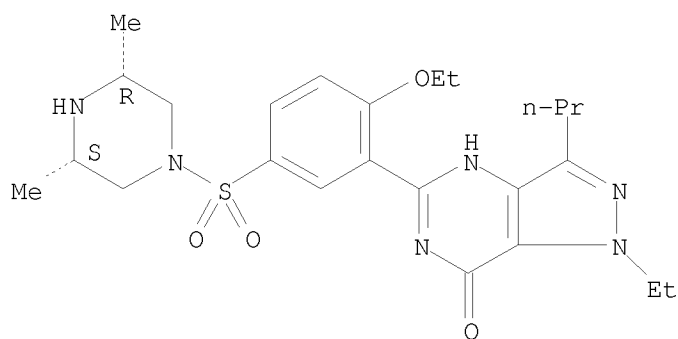
MF C25 H37 N6 O4 S

Relative stereochemistry.



L8 6 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN Piperazine, 1-[[4-ethoxy-3-(1-ethyl-4,7-dihydro-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)phenyl]sulfonyl]-3,5-dimethyl-, (3R,5S)-rel-
 (9CI)
 MF C24 H34 N6 O4 S

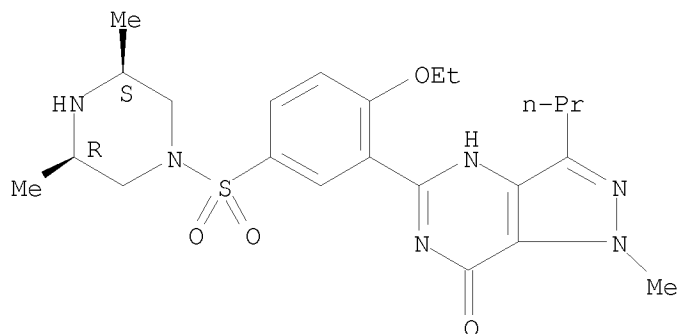
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 6 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 5-[5-[[3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel-
 MF C23 H32 N6 O4 S

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

172.55

348.73

FILE 'CAPLUS' ENTERED AT 10:07:26 ON 23 OCT 2007

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FILE LAST UPDATED: 22 Oct 2007 (20071022/ED)

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=> s 18

L9 8 L8

=> d 19 1-8 ibib abs hitstr

L9 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2007:828226 CAPLUS

TITLE: Use of liquid chromatography-mass spectrometry and a chemical cleavage reaction for the structure elucidation of a new sildenafil analogue detected as an adulterant in an herbal dietary supplement

AUTHOR(S): Reepmeyer, John C.; Woodruff, Jeffrey T.

CORPORATE SOURCE: Division of Pharmaceutical Analysis, US Food and Drug Administration, St. Louis, MO, 63101, USA
SOURCE: Journal of Pharmaceutical and Biomedical Analysis (2007), 44(4), 887-893
CODEN: JPBADA; ISSN: 0731-7085
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An herbal dietary supplement, marketed as a natural product for the enhancement of sexual function, was analyzed by HPLC with photodiode array and mass spectral detection and found to contain a compound related to the synthetic phosphodiesterase-5 (PDE-5) inhibitors. Based on UV spectra, mass spectra and direct infusion MSn, the structure of the compound was tentatively identified as a sildenafil analog in which the sulfonyl group had been replaced with an acetyl group. This new analog is similar to acetildenafil, a previously reported sildenafil analog, but differs in that it contains an N-Me group where acetildenafil contains an N-Et group. The structure of the unknown was unequivocally established by chemical cleavage of the phenacylamine group of the mol. to generate N-methylpiperazine; other cleavage products matched those generated from acetildenafil. Since the new compound has one less CH2 group than acetildenafil, it was named nor-acetildenafil.

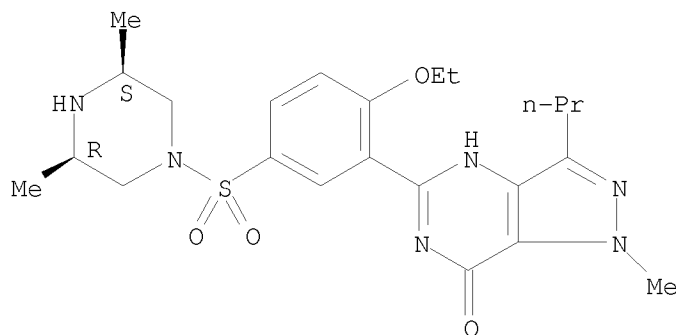
IT 496835-35-9

RL: ANT (Analyte); ANST (Analytical study)
(use of liquid chromatog.-mass spectrometry and a chemical cleavage reaction for structure elucidation of a new sildenafil analog detected as an adulterant in an herbal dietary supplement)

RN 496835-35-9 CAPLUS

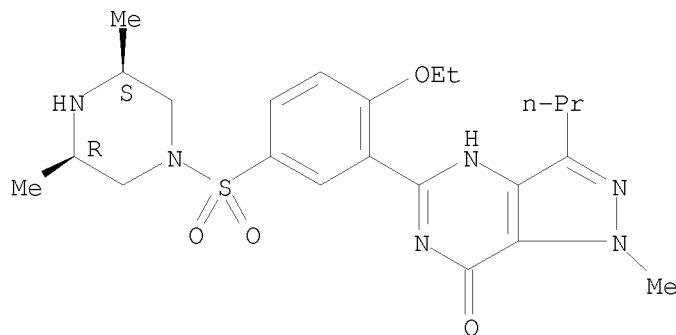
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 5-[5-[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



PATENT INFORMATION:

Relative stereochemistry.



L9 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:422822 CAPLUS
DOCUMENT NUMBER: 147:63259
TITLE: Liquid chromatography tandem mass spectrometry assay
to determine the pharmacokinetics of aildenafil in
human plasma
AUTHOR(S): Wang, Jiang; Jiang, Yao; Wang, Yingwu; Zhao, Xia; Cui,
Yimin; Gu, Jingkai
CORPORATE SOURCE: Research Center for Drug Metabolism, College of Life
Science, Jilin University, Changchun, 130023, Peop.
Rep. China
SOURCE: Journal of Pharmaceutical and Biomedical Analysis
(2007), 44(1), 231-235
CODEN: JPBADA; ISSN: 0731-7085
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A simple, sensitive and specific liquid chromatog./tandem mass spectrometry
method for the quantitation of aildenafil, a new phosphodiesterase V
inhibitor, in human plasma is presented. The analyte and internal standard,
sildenafil, were extracted by a one-step liquid-liquid extraction in alkaline
conditions

and separated on a C18 column using ammonia:10mM ammonium acetate buffer:methanol (0.1:15:85, volume/volume/v) as the mobile phase. The detection by an API 4000 triple quadrupole mass spectrometer in multiple-reaction monitoring mode was completed within 2.5 min. The calibration curve exhibited a linear dynamic range of 0.05 - 100 ng/mL with a 10 pg/mL limit of detection. The intra- and inter-day precisions measured as relative standard deviation were within 8.04% and 5.72%, resp. This method has been used in a pharmacokinetic study of aildenafil in healthy male volunteers each given an oral administration of one of the three dosages.

IT 496835-35-9, Aildenafil

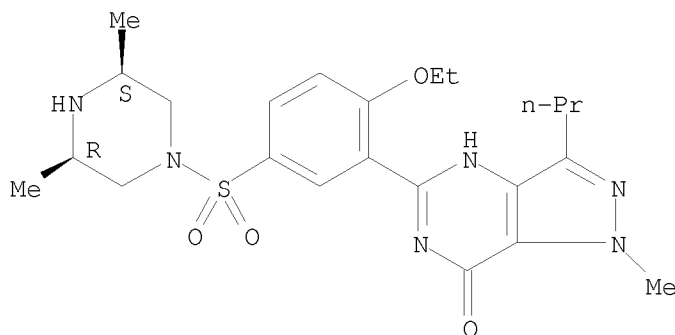
RL: BSU (Biological study, unclassified); PKT (Pharmacokinetics); BIOL (Biological study)

(liquid chromatog. tandem mass spectrometry assay to determine the pharmacokinetics of aildenafil in human plasma)

RN 496835-35-9 CAPLUS

CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2007:345344 CAPLUS

DOCUMENT NUMBER: 147:39501

TITLE: Structure elucidation of a novel analogue of sildenafil detected as an adulterant in an herbal dietary supplement

AUTHOR(S): Reepmeyer, John C.; Woodruff, Jeffrey T.; 'Avignon, D. Andre

CORPORATE SOURCE: Division of Pharmaceutical Analysis, US Food and Drug Administration, St. Louis, MO, 63101, USA

SOURCE: Journal of Pharmaceutical and Biomedical Analysis (2007), 43(5), 1615-1621
CODEN: JPBADA; ISSN: 0731-7085

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new analog of sildenafil was detected in an herbal dietary supplement, which was sold over the internet and promoted as a product for the enhancement of sexual performance. The structure of the compound was established using LC-MS, UV spectroscopy, MS-MS, and NMR. In addition, the compound was cleaved at its sulfonamide S-N bond yielding a sulfonic acid and an amine, which were independently characterized using LC-MS, GC-MS, and derivatization. The compound, named methisosildenafil, is a novel

synthetic analog of sildenafil in which the N-methylpiperazine moiety has been replaced with 2,6-dimethylpiperazine.

IT 496835-35-9, Methisosildenafil

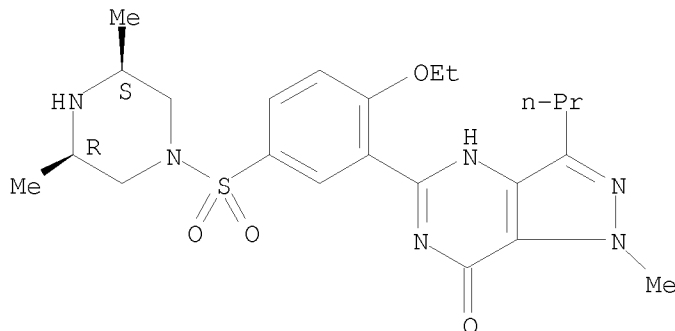
RL: ANT (Analyte); ANST (Analytical study)

(structure elucidation of a novel analog of sildenafil detected as an adulterant in an herbal dietary supplement)

RN 496835-35-9 CAPLUS

CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:570896 CAPLUS

DOCUMENT NUMBER: 143:97390

TITLE: Preparation of pyrazolopyrimidinethione derivatives for treatment of impotence

INVENTOR(S): Li, Shuxin; Ren, Jianping; Zhao, Yanjin; Lv, QiuJun; Guo, Jinhua

PATENT ASSIGNEE(S): The Institute of Radiation Medicine, Academy of Military Medical Sciences Pla, Peop. Rep. China

SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

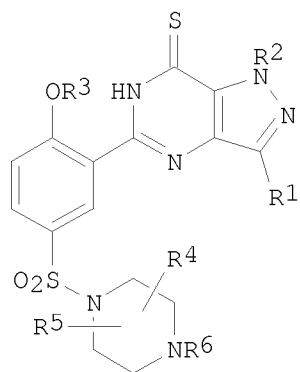
LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

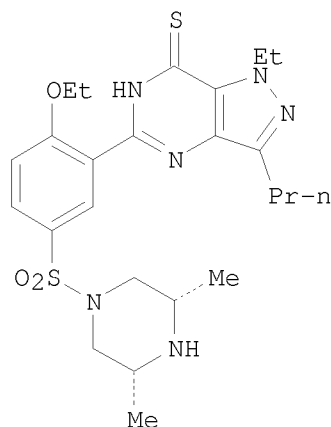
PATENT INFORMATION:

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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CN 1629163	A	20050622	CN 2003-10118481	20031218
EP 1695976	A1	20060830	EP 2004-797343	20041118

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS
 IN 2006MN00737 A 20070330 IN 2006-MN737 20060623
 US 2007219220 A1 20070920 US 2007-583335 20070215
 PRIORITY APPLN. INFO.: CN 2003-10118481 A 20031218
 WO 2004-CN1312 W 20041118
 OTHER SOURCE(S): CASREACT 143:97390; MARPAT 143:97390
 GI



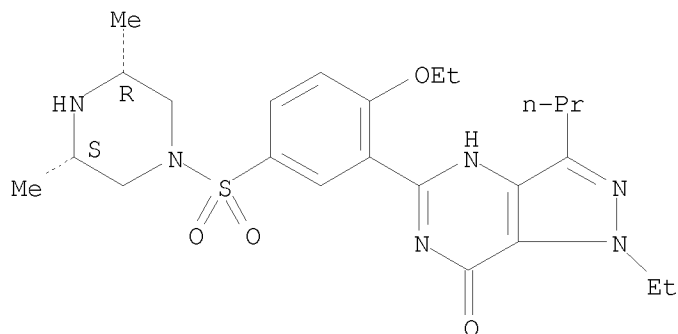
I



II

- AB Title compds. represented by the formula I [wherein R1-R3 = independently ((cyclo)alkoxy)alkyl, alkenyl or aryl; R4 = alkyl, alkenyl, (cyclo)alkoxy, aryl; R5 = H, alkyl, alkenyl, (cyclo)alkoxy, aryl; R6 = H, (cyclo)alkyl, alkenyl, alkylcarbonyl; and pharmaceutically acceptable salts or solvates thereof] were prepared for treatment of impotence. For example, II was given in a multi-step synthesis starting from 4-amino-1-ethyl-3-propylpyrazole-5-carboxamide. I showed enhanced erectile response in rats similar to that of Sildenafil. Thus, I and their pharmaceutical compns. are useful for the treatment of impotence and sexlessness, having high selectivity over PDE V, long action time, less side reactions, and no side effects of blood pressure decreasing and heart rate increasing.
- IT 856190-55-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of pyrazolopyrimidinethione derivs. for treatment of impotence)
- RN 856190-55-1 CAPLUS
- CN Piperazine, 1-[[4-ethoxy-3-(1-ethyl-4,7-dihydro-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)phenyl]sulfonyl]-3,5-dimethyl-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:476529 CAPLUS

DOCUMENT NUMBER: 143:7736

TITLE: Preparation of piperazine derivatives for treating impotence

INVENTOR(S): Liu, Baoshun; Wang, Maotian

PATENT ASSIGNEE(S): Peop. Rep. China

SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, No pp. given

CODEN: CNXXEV

DOCUMENT TYPE: Patent

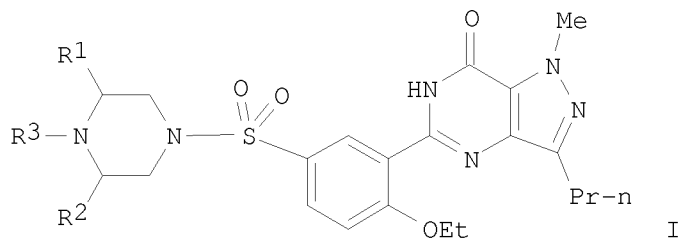
LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

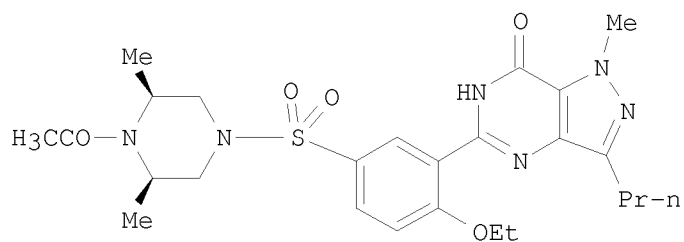
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1517349	A	20040804	CN 2003-100488	20030116
PRIORITY APPLN. INFO.:			CN 2003-100488	20030116
OTHER SOURCE(S):		CASREACT 143:7736; MARPAT 143:7736		

GI



I



II

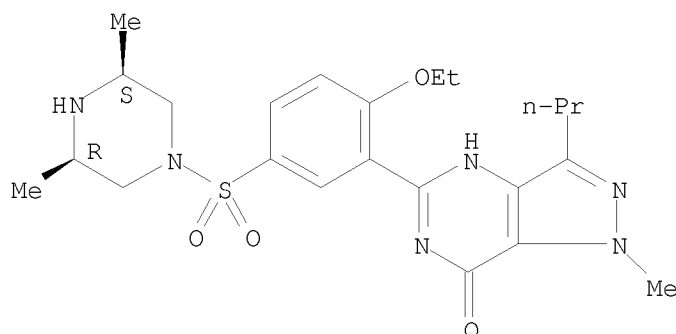
AB The title compds. I [wherein R1 and R2 = independently alkyl; R3 = acyl or dimethyl] or pharmaceutically acceptable salts or isomers thereof are prepared for the treatment of impotence. For example, the compound II was prepared II showed good result in treating impotence in rat.

IT 496835-35-9P
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (drug candidate; preparation of piperazine derivs. for treating impotence)

RN 496835-35-9 CAPLUS

CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel- (CA INDEX NAME)

Relative stereochemistry.

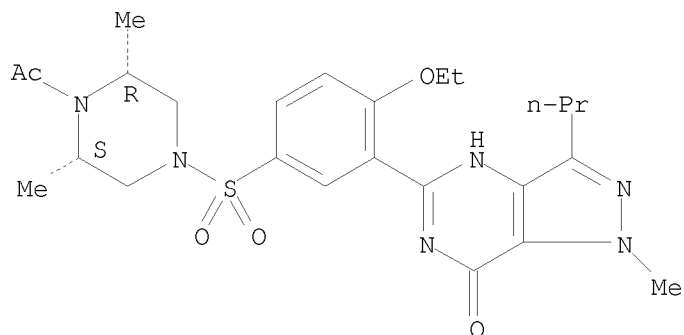


IT 852615-88-4P 852615-89-5P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (drug candidate; preparation of piperazine derivs. for treating impotence)

RN 852615-88-4 CAPLUS

CN Piperazine, 1-acetyl-4-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-2,6-dimethyl-, (2R,6S)-rel- (9CI) (CA INDEX NAME)

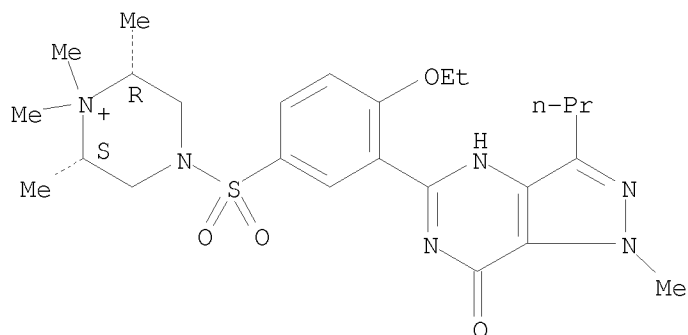
Relative stereochemistry.



RN 852615-89-5 CAPLUS

CN Piperazinium, 4-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-1,1,2,6-tetramethyl-, (2R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L9 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:1009838 CAPLUS

DOCUMENT NUMBER: 142:392422

TITLE: Preparation of fused ring aromatic compounds for treatment of sexual disorders

INVENTOR(S): Lu, Derang; Li, Zhihai

PATENT ASSIGNEE(S): Peop. Rep. China

SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 15 pp.
CODEN: CNXXEV

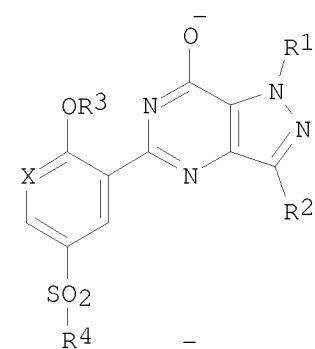
DOCUMENT TYPE: Patent

LANGUAGE: Chinese

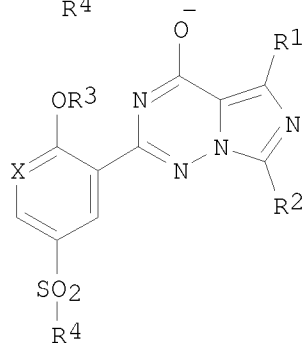
FAMILY ACC. NUM. COUNT: 1

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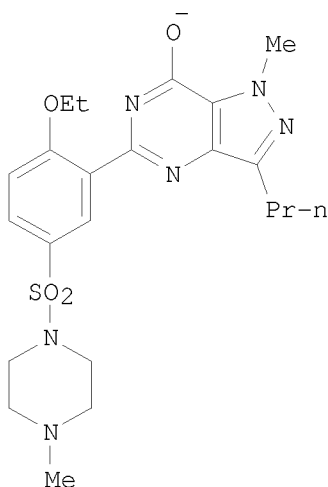
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CN 1472210	A	20040204	CN 2002-138880	20020802
PRIORITY APPLN. INFO.:			CN 2002-138880	20020802
OTHER SOURCE(S):	MARPAT	142:392422		
GI				



I



II



III

AB The title compds. I•N+R7R8R9R10 and II•NR7R8R9R10 [wherein R1 = H, alkyl, haloalkyl, or cycloalkyl; R2 = H, (un)substituted alkyl, haloalkyl, or cycloalkyl; R3 = H, (un)substituted alkyl, haloalkyl, cycloalkyl, alkenyl, or alkynyl; R4 = (un)substituted NH2 or piperazinyl; R7, - R10 = independently aryl or alkyl; X = CH or N] are prepared for the treatment of sexual disorders. For example, the compound III•N+Me3(CH2CH2OH) was prepared in a two-step synthesis in good yield. The title compds. showed strong effect on sexual disorders in rat.

IT 849915-00-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of fused ring aromatic compds. for treatment of sexual disorders)

RN 849915-00-0 CAPLUS

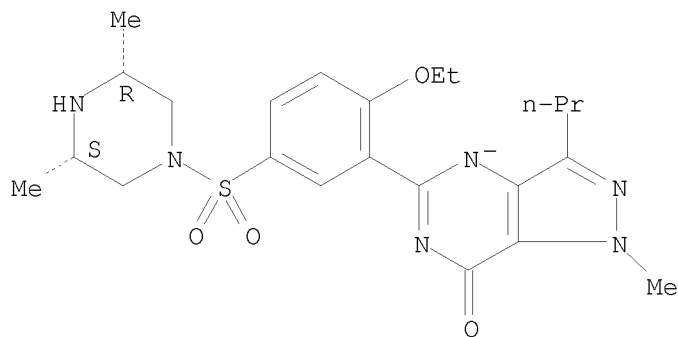
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with rel-(3R,5S)-1-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-3,5-dimethylpiperazine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 849914-99-4

CMF C23 H31 N6 O4 S

Relative stereochemistry.



CM 2

CRN 62-49-7

CMF C5 H14 N O

$\text{Me}_3\text{N}^+\text{CH}_2\text{CH}_2\text{OH}$

IT 496835-35-9P

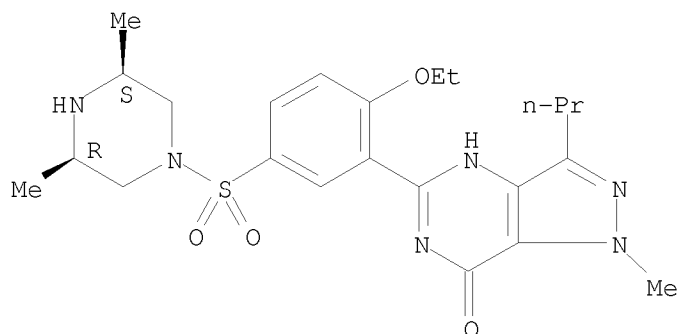
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of fused ring aromatic compds. for treatment of sexual disorders)

RN 496835-35-9 CAPLUS

CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



L9 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:154433 CAPLUS

DOCUMENT NUMBER: 138:153550

TITLE: Preparation of pyrazolopyrimidine derivatives for treatment of impotence

INVENTOR(S): Liu, Baoshun

PATENT ASSIGNEE(S): Peop. Rep. China

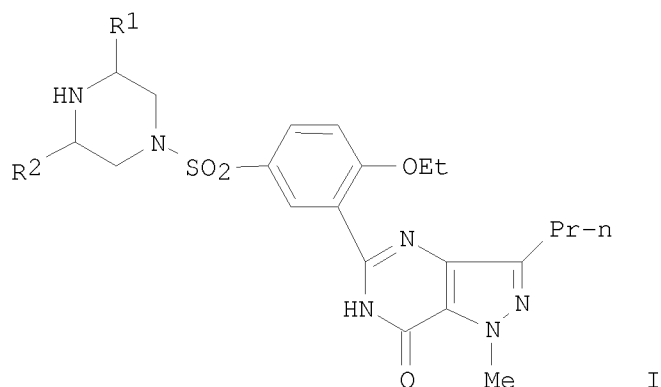
SOURCE: PCT Int. Appl., 20 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Chinese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

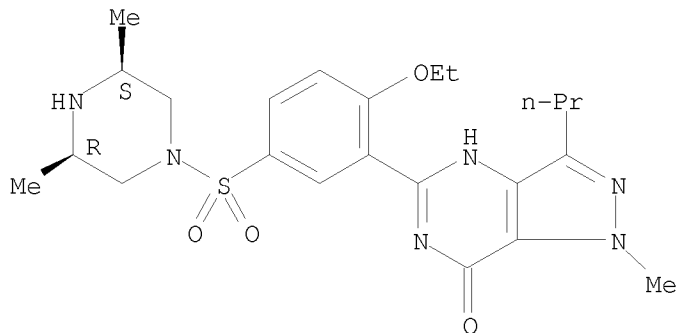
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WO 2003016313	A1	20030227	WO 2002-CN433	20020621
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CN 1393444	A	20030129	CN 2002-100198	20020118
CN 1127506	B	20031112		
CA 2451990	A1	20030227	CA 2002-2451990	20020621
AU 2002323774	A1	20030303	AU 2002-323774	20020621
EP 1400522	A1	20040324	EP 2002-754139	20020621
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2002011025	A	20041019	BR 2002-11025	20020621
JP 2005500381	T	20050106	JP 2003-521235	20020621
NZ 530548	A	20050429	NZ 2002-530548	20020621
RU 2279433	C2	20060710	RU 2004-102513	20020621
HK 1053108	A1	20040402	HK 2003-105310	20030723
US 2004152709	A1	20040805	US 2003-736732	20031216
US 6960592	B2	20051101		
MX 2003PA11929	A	20050307	MX 2003-PA11929	20031218
IN 2003DN02254	A	20060120	IN 2003-DN2254	20031224
ZA 2004000692	A	20041014	ZA 2004-692	20040128
PRIORITY APPLN. INFO.:			CN 2001-129691	A 20010629
			CN 2002-100198	A 20020118
			WO 2002-CN433	W 20020621
OTHER SOURCE(S):			CASREACT 138:153550; MARPAT 138:153550	
GI				



AB Title compound I (R1, R2 = alkyl) and their pharmaceutically acceptable salts or their configuration isomers., useful for treatment of impotence, are prepared Thus, I (R1 = R2 = Me) (II) was prepared in several steps from 2-ethoxybenzoic acid. II showed enhanced erectile response in rats similar to that of sildenafil.

IT 496835-35-9P
 RL: ADV (Adverse effect, including toxicity); IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of pyrazolopyrimidine derivs. for treatment of impotence)
 RN 496835-35-9 CAPLUS
 CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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COST IN U.S. DOLLARS	SINCE FILE	TOTAL	
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FULL ESTIMATED COST	45.45	394.18	
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL	
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CA SUBSCRIBER PRICE	-6.24	-6.24	

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NEWS	3	JAN 16 CAS patent coverage enhanced to include exemplified prophetic substances

NEWS	4	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	5	JAN 28	MARPAT searching enhanced
NEWS	6	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS	7	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS	8	JAN 28	MEDLINE and LMEDLINE reloaded with enhancements
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NEWS	11	FEB 25	IFIREF reloaded with enhancements
NEWS	12	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS	13	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS	14	MAR 31	IFICDB, IFIPAT, and IFIUIDB enhanced with new custom IPC display formats
NEWS	15	MAR 31	CAS REGISTRY enhanced with additional experimental spectra
NEWS	16	MAR 31	CA/CAPplus and CASREACT patent number format for U.S. applications updated
NEWS	17	MAR 31	LPCI now available as a replacement to LDPCI
NEWS	18	MAR 31	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
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NEWS	20	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS	21	APR 28	EMBASE Controlled Term thesaurus enhanced
NEWS	22	APR 28	IMSRESEARCH reloaded with enhancements
NEWS	23	MAY 30	INPAFAMDB now available on STN for patent family searching
NEWS	24	MAY 30	DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS	25	JUN 06	EPFULL enhanced with 260,000 English abstracts
NEWS	26	JUN 06	KOREAPAT updated with 41,000 documents
NEWS	27	JUN 13	USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications
NEWS	28	JUN 19	CAS REGISTRY includes selected substances from web-based collections
NEWS	29	JUN 25	CA/CAPplus and USPAT databases updated with IPC reclassification data
NEWS	30	JUN 30	AEROSPACE enhanced with more than 1 million U.S. patent records
NEWS	31	JUN 30	EMBASE, EMBAL, and LEMBASE updated with additional options to display authors and affiliated organizations
NEWS	32	JUN 30	STN on the Web enhanced with new STN AnaVist Assistant and BLAST plug-in
NEWS	33	JUN 30	STN AnaVist enhanced with database content from EPFULL
NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.			
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COST IN U.S. DOLLARS

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TOTAL

ENTRY

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FULL ESTIMATED COST

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DICTIONARY FILE UPDATES: 30 JUN 2008 HIGHEST RN 1031926-83-6

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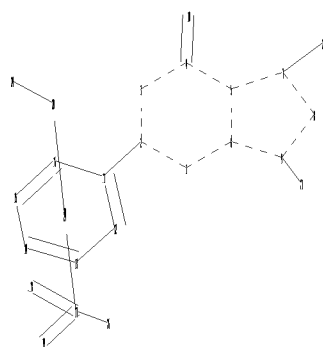
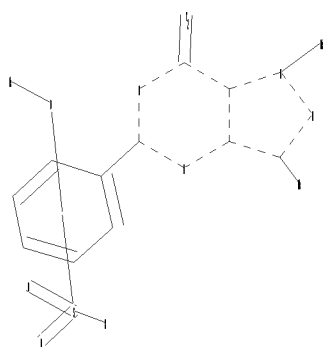
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Uploading C:\Program Files\Stnexp\Queries\10 series\10583335\10583335d.str



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ring nodes :
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ring bonds :
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15-16
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 4-10 5-6 5-7 6-9 7-8 7-22 8-9 9-21 17-26 17-18
17-19 20-24
exact bonds :
2-11
normalized bonds :
11-12 11-16 12-13 13-14 14-15 15-16
isolated ring systems :
containing 1 : 11 :

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G1:H,Ak,Cb

G2:O,S

Match level :

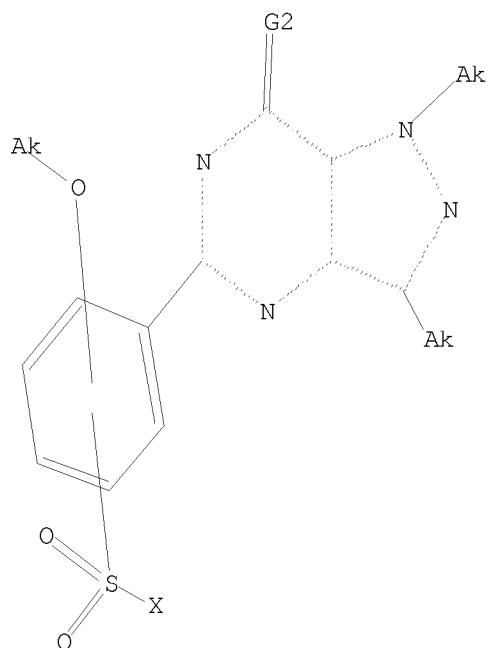
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20:CLASS 21:CLASS 22:CLASS 24:CLASS 26:CLASS 28:Atom 29:Atom

L1 STRUCTURE UPLOADED

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L1 HAS NO ANSWERS

L1 STR



G1 H,Ak,Cb

G2 O,S

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS

1 ANSWERS

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BATCH **COMPLETE**

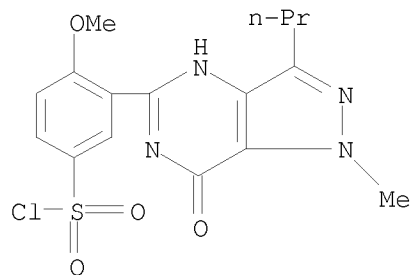
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PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> d scan

L2 1 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN Benzenesulfonyl chloride, 3-(6,7-dihydro-1-methyl-7-oxo-3-propyl-1H-
 pyrazolo[4,3-d]pyrimidin-5-yl)-4-methoxy-
 MF C16 H17 Cl N4 O4 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

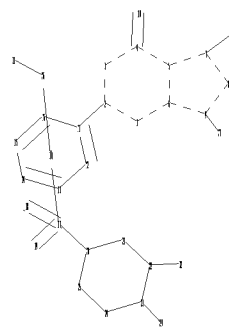
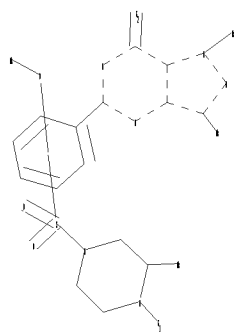
ALL ANSWERS HAVE BEEN SCANNED

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 FULL SCREEN SEARCH COMPLETED - 46 TO ITERATE

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 SEARCH TIME: 00.00.01

L3 24 SEA SSS FUL L1

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ring nodes :
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chain bonds :
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ring bonds :
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15-16 20-21 20-25 21-22 22-23 23-24 24-25
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exact bonds :
2-11
normalized bonds :
11-12 11-16 12-13 13-14 14-15 15-16

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isolated ring systems :
containing 1 : 11 :

G1:H,Ak,Cb

G2:O,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS 28:CLASS
29:CLASS 31:CLASS 32:CLASS 35:Atom 36:Atom

L4 STRUCTURE UPLOADED

=> d 14

L4 HAS NO ANSWERS

L4 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 60 TO ITERATE

100.0% PROCESSED 60 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

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BATCH **COMPLETE**

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PROJECTED ANSWERS: 1 TO 80

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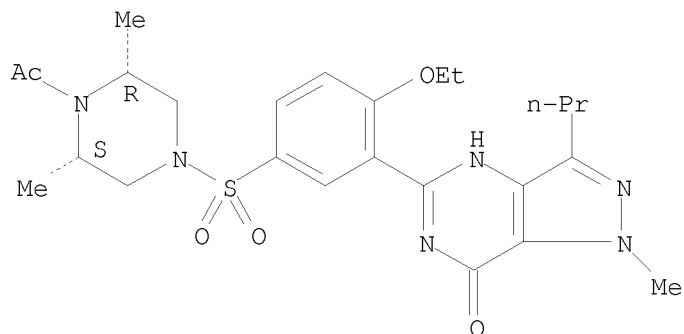
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L5 1 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 5-[5-[(3R,5S)-4-acetyl-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel-

MF C25 H34 N6 O5 S

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

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L6 13 SEA SSS FUL L4

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FILE 'CAPLUS' ENTERED AT 16:23:57 ON 01 JUL 2008
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FILE COVERS 1907 - 1 Jul 2008 VOL 149 ISS 1
 FILE LAST UPDATED: 30 Jun 2008 (20080630/ED)

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L9          22 L3(L) RACT+NT/RL

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has been deleted. To see the L-numbers currently defined in this
session, enter DISPLAY HISTORY at an arrow prompt (=>).

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L11          4 L6(L) PREP+NT/RL

=> s 17 and 110
L12          2 L7 AND L10

=> s 19 and 111
L13          2 L9 AND L11

=> d 113 1-2 ibib hitstr

L13 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:570896 CAPLUS
DOCUMENT NUMBER: 143:97390
TITLE: Preparation of pyrazolopyrimidinethione derivatives
for treatment of impotence
INVENTOR(S): Li, Shuxin; Ren, Jianping; Zhao, Yanjin; Lv, Qiuju;
Guo, Jinhua
PATENT ASSIGNEE(S): The Institute of Radiation Medicine, Academy of
Military Medical Sciences Pla, Peop. Rep. China
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

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WO 2005058899	A1	20050630	WO 2004-CN1312	20041118
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 EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO,
 SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
 NE, SN, TD, TG

CN 1629163	A	20050622	CN 2003-10118481	20031218
EP 1695976	A1	20060830	EP 2004-797343	20041118
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US 20070219220	A1	20070920	US 2007-583335	20070215
PRIORITY APPLN. INFO.:			CN 2003-10118481	A 20031218
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OTHER SOURCE(S): CASREACT 143:97390; MARPAT 143:97390

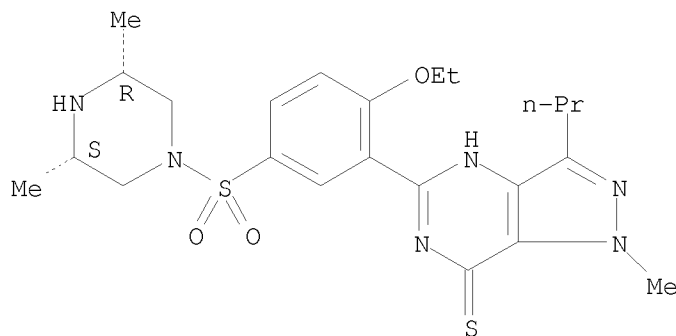
IT 856190-47-1P

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of pyrazolopyrimidinethione derivs. for treatment of impotence)

RN 856190-47-1 CAPLUS

CN 7H-Pyrazolo[4,3-d]pyrimidine-7-thione, 5-[5-[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel-
 (CA INDEX NAME)

Relative stereochemistry.



IT 856190-48-2P 856190-49-3P 856190-50-6P

856190-51-7P 856190-56-2P

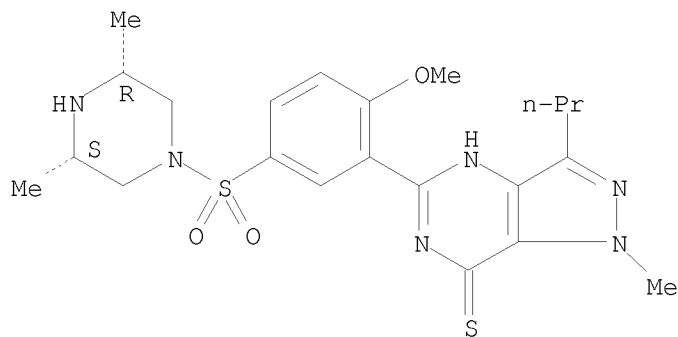
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrazolopyrimidinethione derivs. for treatment of impotence)

RN 856190-48-2 CAPLUS

CN 7H-Pyrazolo[4,3-d]pyrimidine-7-thione, 5-[5-[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-methoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel-
 (CA INDEX NAME)

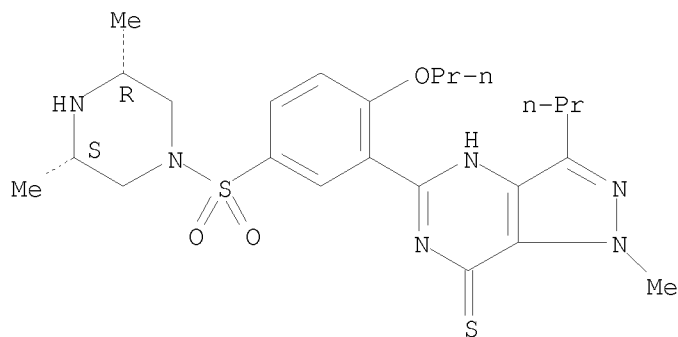
Relative stereochemistry.



RN 856190-49-3 CAPLUS

CN 7H-Pyrazolo[4,3-d]pyrimidine-7-thione, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-propoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel- (CA INDEX NAME)

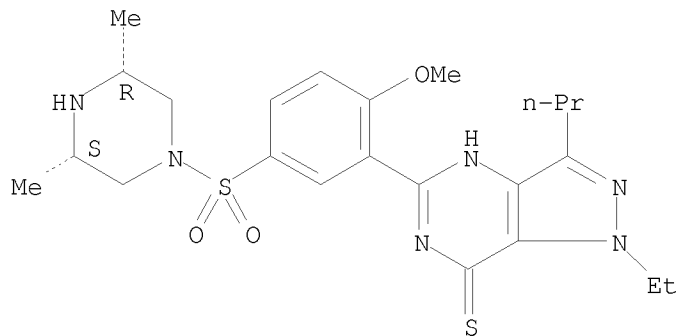
Relative stereochemistry.



RN 856190-50-6 CAPLUS

CN 7H-Pyrazolo[4,3-d]pyrimidine-7-thione, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-methoxyphenyl]-1-ethyl-1,6-dihydro-3-propyl-, rel- (CA INDEX NAME)

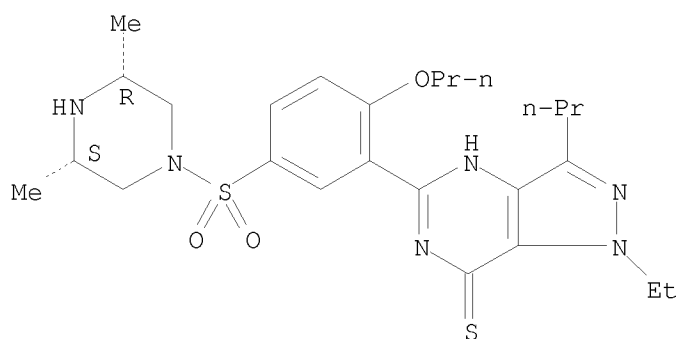
Relative stereochemistry.



RN 856190-51-7 CAPLUS

CN 7H-Pyrazolo[4,3-d]pyrimidine-7-thione, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-propoxyphenyl]-1-ethyl-1,6-dihydro-3-propyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



RN 856190-56-2 CAPLUS

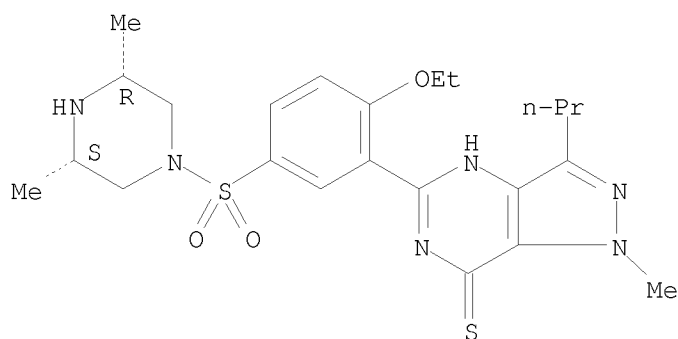
CN 7H-Pyrazolo[4,3-d]pyrimidine-7-thione, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel-, 2-hydroxy-1,2,3-propanetricarboxylate (1:1) (CA INDEX NAME)

CM 1

CRN 856190-47-1

CMF C23 H32 N6 O3 S2

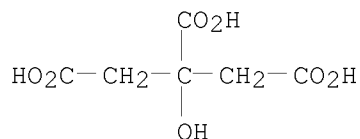
Relative stereochemistry.



CM 2

CRN 77-92-9

CMF C6 H8 O7



IT 139756-35-7P 479074-05-0P 479074-07-2P

856190-53-9P 856190-55-1P

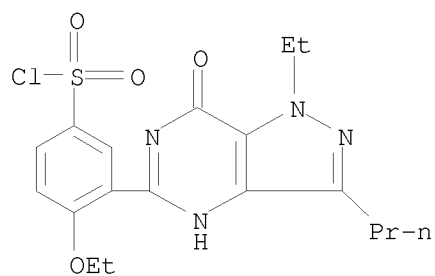
RL: RCT (Reactant); SPN (Synthetic preparation);

PREP (Preparation); RACT (Reactant or reagent)

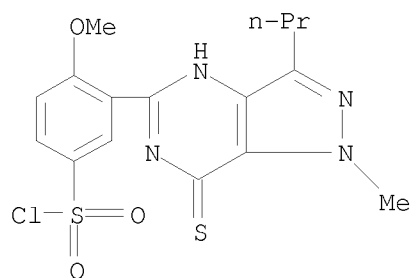
(preparation of pyrazolopyrimidinethione derivs. for treatment of impotence)

RN 139756-35-7 CAPLUS

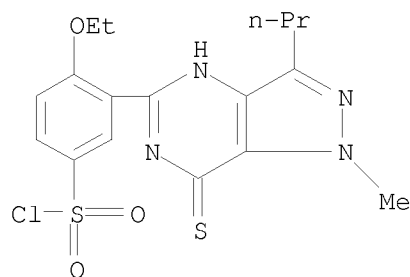
RN Benzenesulfonyl chloride, 4-ethoxy-3-(1-ethyl-4,7-dihydro-7-oxo-3-propyl-
CN 1H-pyrazolo[4,3-d]pyrimidin-5-yl)- (9CI) (CA INDEX NAME)



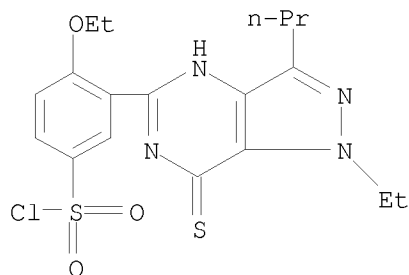
RN 479074-05-0 CAPLUS
CN Benzenesulfonyl chloride, 3-(6,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-
pyrazolo[4,3-d]pyrimidin-5-yl)-4-methoxy- (CA INDEX NAME)



RN 479074-07-2 CAPLUS
CN Benzenesulfonyl chloride, 3-(6,7-dihydro-1-methyl-3-propyl-7-thioxo-1H-
pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxy- (CA INDEX NAME)



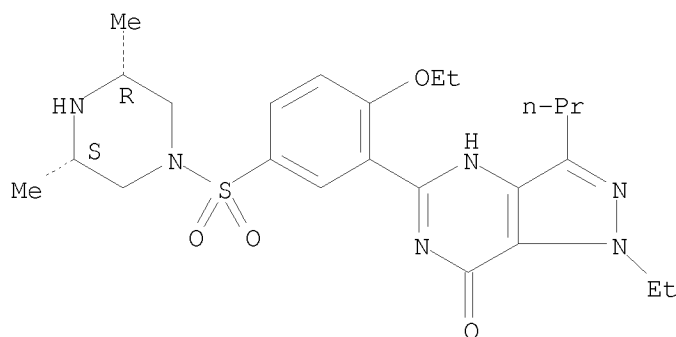
RN 856190-53-9 CAPLUS
CN Benzenesulfonyl chloride, 4-ethoxy-3-(1-ethyl-6,7-dihydro-3-propyl-7-
thioxo-1H-pyrazolo[4,3-d]pyrimidin-5-yl)- (CA INDEX NAME)



RN 856190-55-1 CAPLUS

CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1-ethyl-1,6-dihydro-3-propyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:1009838 CAPLUS

DOCUMENT NUMBER: 142:392422

TITLE: Preparation of fused ring aromatic compounds for treatment of sexual disorders

INVENTOR(S): Lu, Derang; Li, Zhihai

PATENT ASSIGNEE(S): Peop. Rep. China

SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 15 pp.

CODEN: CNXXEV

DOCUMENT TYPE: Patent

LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1472210	A	20040204	CN 2002-138880	20020802
PRIORITY APPLN. INFO.:			CN 2002-138880	20020802
OTHER SOURCE(S):			MARPAT 142:392422	
IT 849915-00-0P				

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);
THU (Therapeutic use); BIOL (Biological study); PREP (Preparation)
; USES (Uses)

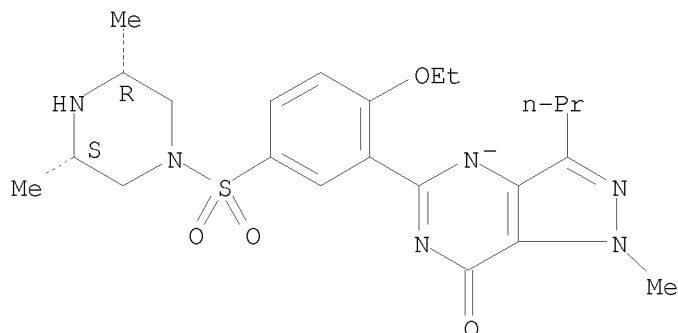
(preparation of fused ring aromatic compds. for treatment of sexual disorders)

RN 849915-00-0 CAPLUS
 CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one (1:1) (CA INDEX NAME)

CM 1

CRN 849914-99-4
 CMF C23 H31 N6 O4 S

Relative stereochemistry.

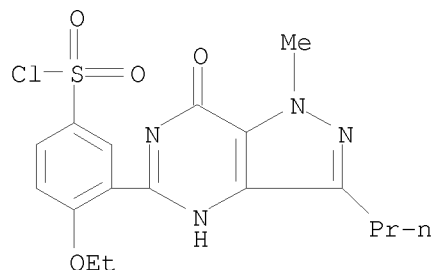


CM 2

CRN 62-49-7
 CMF C5 H14 N O

$\text{Me}_3\text{N}^+-\text{CH}_2-\text{CH}_2-\text{OH}$

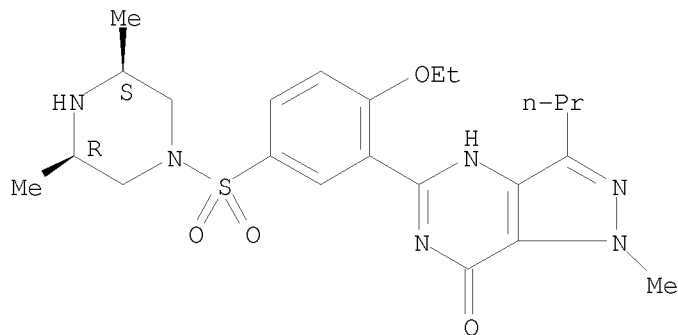
IT 139756-22-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of fused ring aromatic compds. for treatment of sexual disorders)
 RN 139756-22-2 CAPLUS
 CN Benzenesulfonyl chloride, 3-(6,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxy- (CA INDEX NAME)



IT 496835-35-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of fused ring aromatic compds. for treatment of sexual disorders)

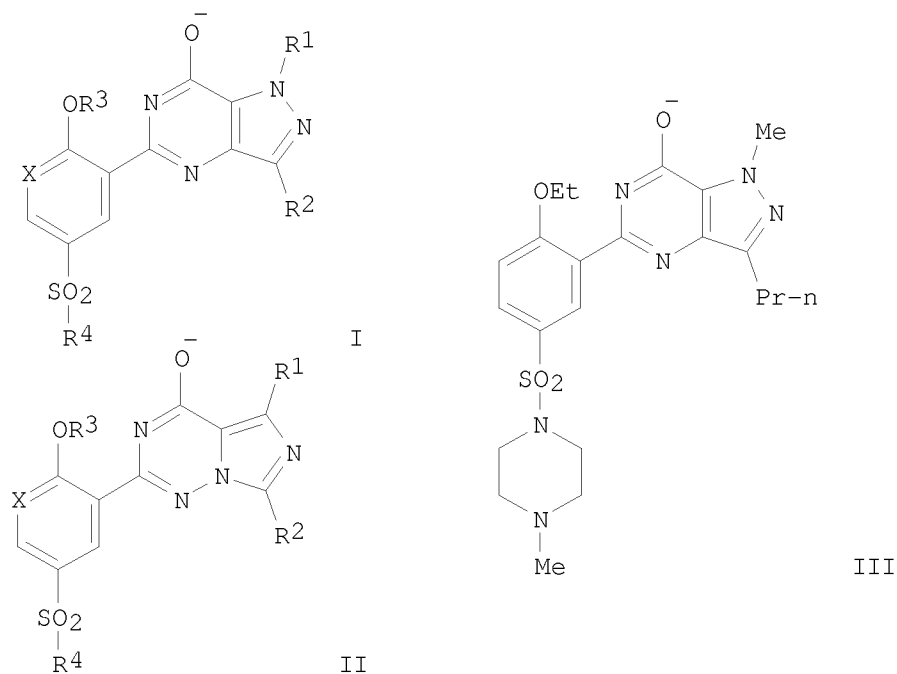
RN 496835-35-9 CAPLUS
 CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel-
 (CA INDEX NAME)

Relative stereochemistry.



=> d 113 2 abs

L13 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
 GI



AB The title compds. I•N+R7R8R9R10 and II•NR7R8R9R10 [wherein R1 = H, alkyl, haloalkyl, or cycloalkyl; R2 = H, (un)substituted alkyl, haloalkyl, or cycloalkyl; R3 = H, (un)substituted alkyl, haloalkyl, cycloalkyl, alkenyl, or alkynyl; R4 = (un)substituted NH2 or piperazinyl; R7, - R10 =

independently aryl or alkyl; X = CH or N] are prepared for the treatment of sexual disorders. For example, the compound III•N+Me3(CH2CH2OH) was prepared in a two-step synthesis in good yield. The title compds. showed strong effect on sexual disorders in rat.

=> log hold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

27.36

384.29

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-0.80

-0.80

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 16:41:07 ON 01 JUL 2008